3-Methoxybutyl acetate

	,	•	
4435-53-4	DTX	SID20521	0

Model Performance

Model	Data
iviodei	Dala

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 164 °C

Global applicability domain: Inside

Local applicability domain index: 7.26e-01

Confidence level: 8.04e-01

Nearest Neighbors from the Training Set

Image not found

Acetic acid, ethoxy-, ethyl ester

Measured: 158 Predicted: 156

Image not found

Ethyl orthoformate

Measured: 143 Predicted: 149

Image not found

Acetic acid, chloro-, butyl ester

Measured: 183 Predicted: 175

Image not found

Ethyl 4-chlorobutyrate

Measured: 184 Predicted: 175